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# DOE's Fundamental Science Underpinning Energy Storage



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U.S. DEPARTMENT OF ENERGY



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John Vetrano  
Office of Basic Energy Sciences



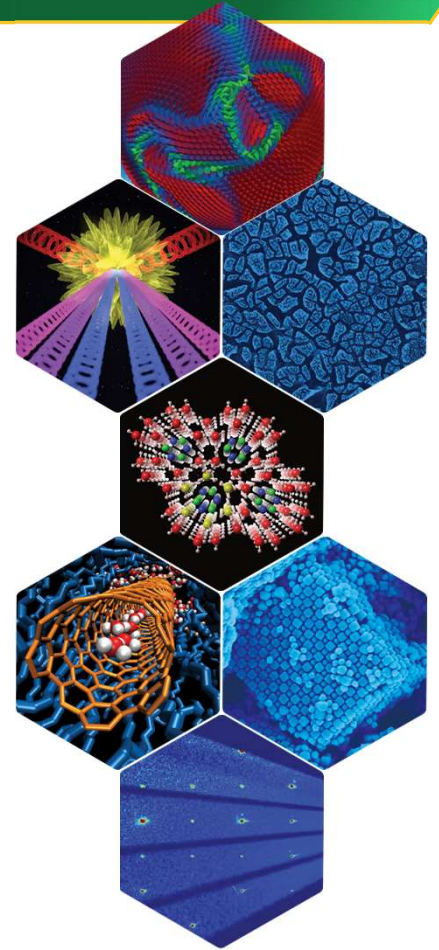
ENERGY STORAGE  
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U.S. DEPARTMENT OF ENERGY

# Basic Energy Sciences Mission

To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels

## BES fulfills its mission through:

- ▶ Supporting **basic research** to discover new materials and design new chemical processes that underpin a broad range of energy technologies
  - ❖ **Critical role in clean energy research**
- ▶ Operating **world-class scientific user facilities** in x-ray, neutron, and electron beam scattering as well as in nanoscale research
- ▶ Managing **construction and upgrade projects** to maintain **world-leading** scientific user facilities



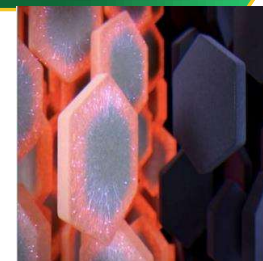


# Fundamental Research for Energy is Supported in Each of the Major BES Research Modalities

Increasing scope and size

## ► Core Research

Single investigators (~\$150K/year) and small groups (\$500K-\$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics from the annual SC FOA, through their national lab, or through special topic FOAs; typically, 3-year awards. Annual SC FOA open year-round. Includes SC Early Career Research Program.



Lithium Diffusion

## ► Energy Frontier and Energy Earthshot Research Centers

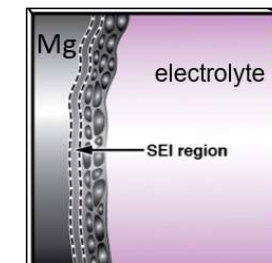
\$2-4 million/year research centers for 4-year award terms; focus on fundamental research described in Basic Research Needs Workshop reports.



Polymer Electrolytes

## ► Energy Storage & Fuels from Sunlight Energy Innovation Hubs

Large-team research awards (5-year terms; \$8-25M/year) focus on topics that have proven challenging for traditional funding modalities and for which success could be transformative to science and technology. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.



New Battery Chemistries

# Overcoming S&T Challenges to Meet Transformative Energy Goals

DOE's Energy Earthshots™ target the remaining, major RD&D breakthroughs we know we must achieve in the next decade to solve the climate crisis and reach our 2050 net-zero carbon goals.

## Hydrogen Shot



1 Dollar



1 Kilogram



1 Decade

## Long Duration Storage Shot



Reduce storage costs by 90%...

...in storage systems That deliver 10+ hours of duration

...in 1 decade

\*from a 2020 Li-Ion baseline

## Carbon Negative Shot



<100 Dollars



1 Ton



1 Decade

## Clean Fuels and Products



85% Reduction



2035

## Enhanced Geothermal Shot



90% Reduction



2035

## Floating Offshore Wind Shot



>70% Reduction



2035

## Industrial Heat Shot



85% Reduction



2035

<https://www.energy.gov/policy/energy-earthshots-initiative>

# SC Energy Earthshots Initiative

Apr. 2023

- ▶ Addresses key research challenges at the interface between basic research and applied R&D to realize DOE Energy Earthshots stretch goals.
- ▶ BES, ASCR, and BER issued an FY 2023 lab announcement for Energy Earthshot Research Centers (EERCs).
  - ❖ Modeled on EFRCs, EERCs will support large multi-investigator, multi-disciplinary, and multi-institution (academic, national laboratory, industrial) teams to advance foundational knowledge and enabling capabilities in experimental & computational chemical/materials sciences to address Earthshot goals.
  - ❖ Closely coordinated with the Energy Technology Offices and existing research consortia/demonstration projects, to establish teams that span the R&D continuum and accelerate both science and technologies—providing a strong bridge between BES and technology research.
- ▶ EERCs are complemented with foundational science, small group awards.
  - ❖ Focus on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy Earthshot goals.

## Enhanced Geothermal Shot



90% Reduction



2035

## Floating Offshore Wind Shot



>70% Reduction



2035

## Industrial Heat Shot



85% Reduction



2035

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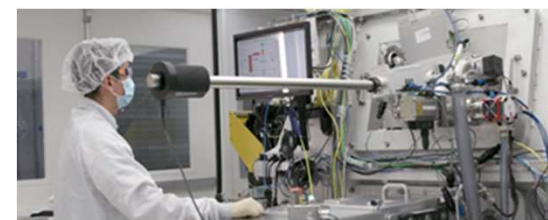
1 Decade

# FY 2024 Request: SC Energy Earthshots Initiative

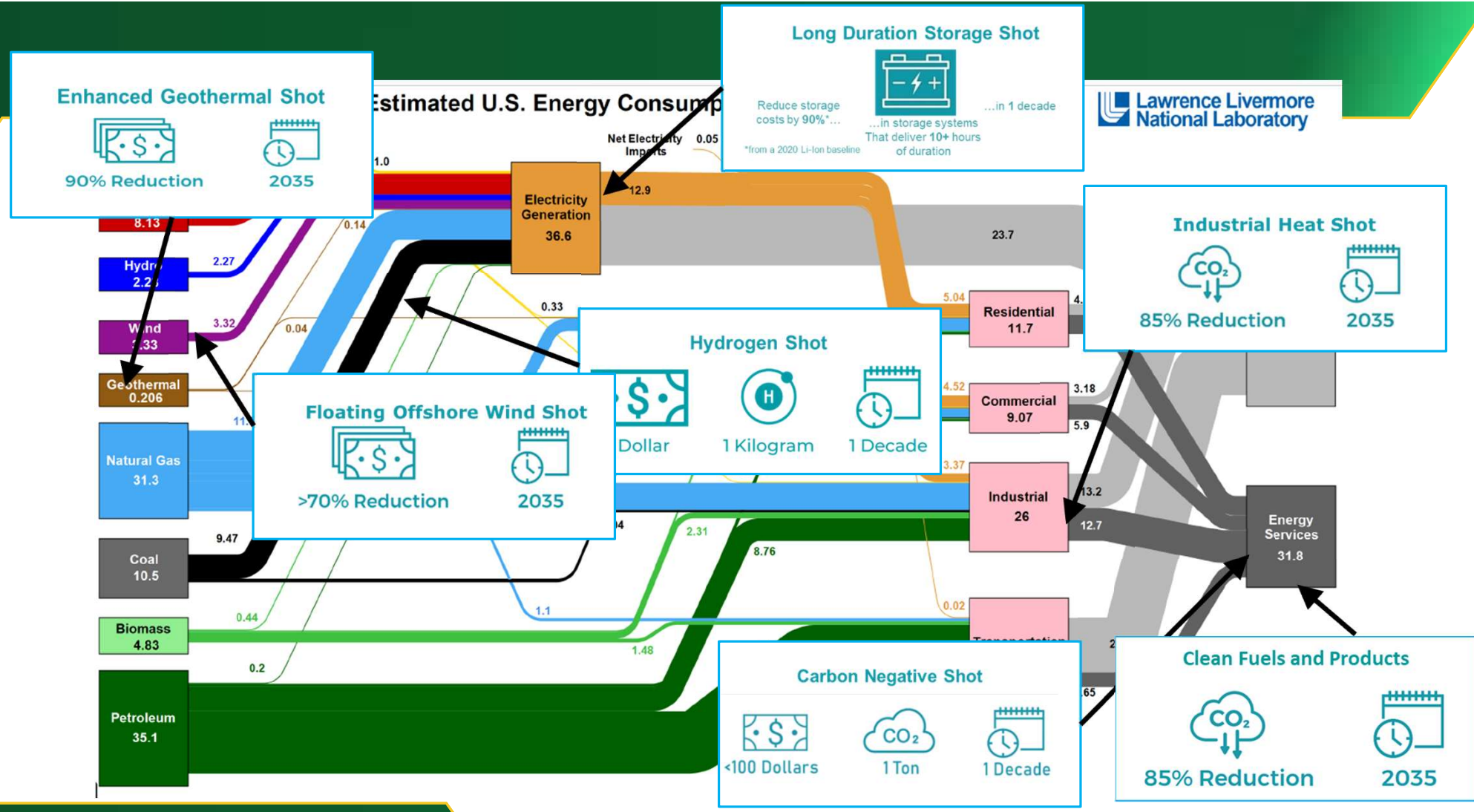
Joint initiative between BES, ASCR, and BER to address key research challenges at the interface between basic research and applied R&D to realize DOE Energy Earthshots stretch goals. (+\$35M; +\$75M for all of SC):

Two complementary programs:

- Energy Earthshot Research Centers (EERCs): Multi-disciplinary, multi-institutional teams led by DOE laboratories focused on key research challenges at the interface of basic and applied R&D.
- Scientific Foundations for Energy Earthshots: Small group awards led by academic or private sector institutions focused on use-inspired foundational science addressing knowledge gaps limiting achievement of Earthshot goals.

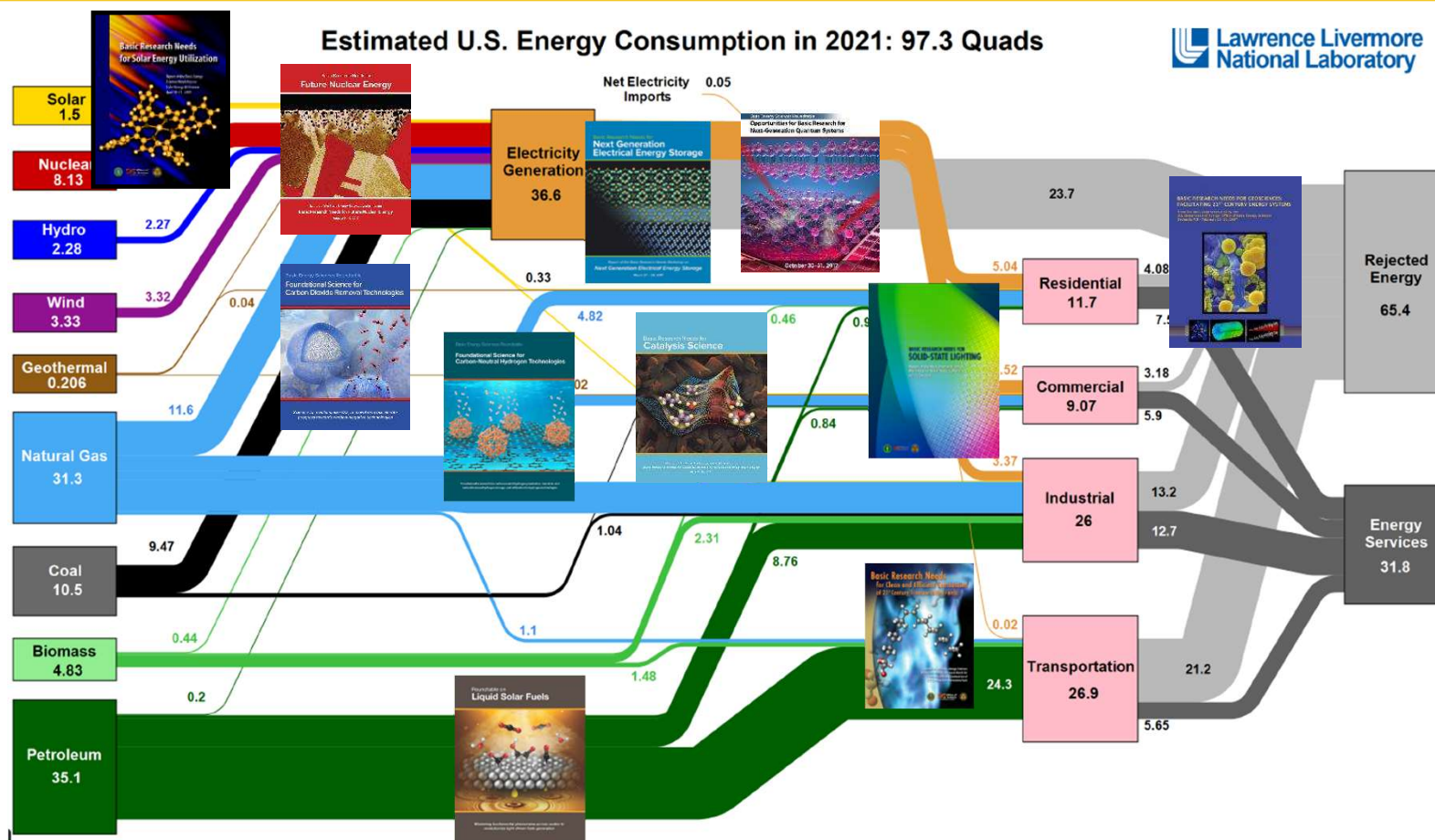








# Basic Research Needs Reports Address Many Energy Topics



# Basic Research Needs Workshop on Next-Generation Electrical Energy Storage

## **Tune functionality of materials and chemistries to enable holistic design for energy storage**

*How can we understand the functionality of materials sufficiently to anticipate their behavior in electrochemical configurations? How can these insights inform the design of chemistries, materials, and structures for future energy storage?*

## **Link complex electronic, electrochemical, and physical phenomena across time and space**

*What modeling frameworks can express the spatiotemporal evolution of material-chemical systems across varying spatial and temporal scales?*

*How can models inform experimental strategies to provide insight on electrochemical phenomena?*

## **Control and exploit the complex interphase region formed at dynamic interfaces**

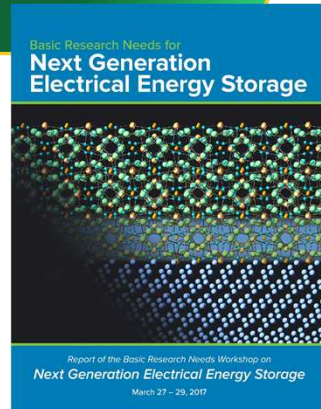
*Can we characterize the chemical and material reactions and behaviors that comprise dynamic interfaces? How can interfaces be designed and synthesized to enhance storage performance and/or mitigate degradation?*

## **Revolutionize energy storage performance through innovative assemblies of matter**

*What strategies can we use to exploit high-capacity electrode materials and higher voltage electrolyte chemistries while ensuring reliable cycling? What approaches are needed to perform design, characterization, and simulation at the mesoscale?*

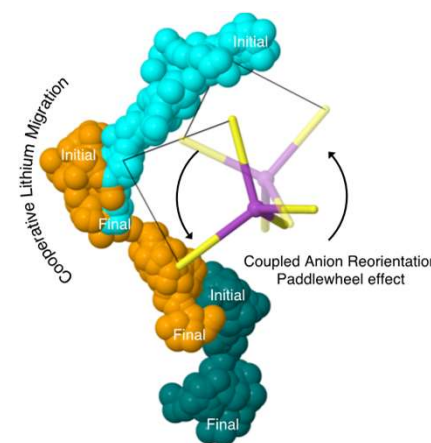
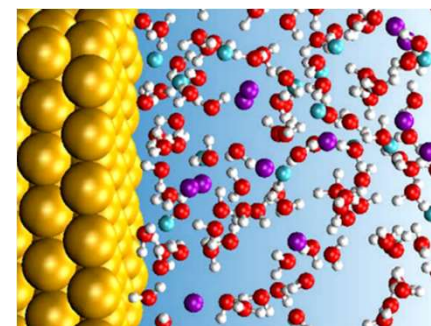
## **Promote self-healing and eliminate detrimental chemistries to extend lifetime and improve safety**

*What drives the key degradation and failure mechanisms? How can these, and possible mitigation strategies, be revealed through modeling and characterization of representative and model systems?*



# BES Support for Energy Storage Research

- ▶ Fundamental research underpinning electrical energy storage - anodes, cathodes, electrolytes, interfaces, flow batteries and membranes, as well as data and software in the Materials Project.
- ▶ The Batteries and Energy Storage Hub Program focuses on science for next-generation batteries for transportation and grid storage; activities are explicitly tailored to link science and technology communities.
  - ❖ Joint Center for Energy Storage Research (JCESR), 2012-2023
  - ❖ FY2023 Re-competition underway (2-3 awards anticipated)
- ▶ Six Energy Frontier Research Centers are focused on basic research directly linked to understanding and advancing energy storage concepts.
- ▶ >40 university grants and national labs field work proposals support a wide range of basic science related to energy storage, including use of advanced characterization and computing at Office of Science user facilities.

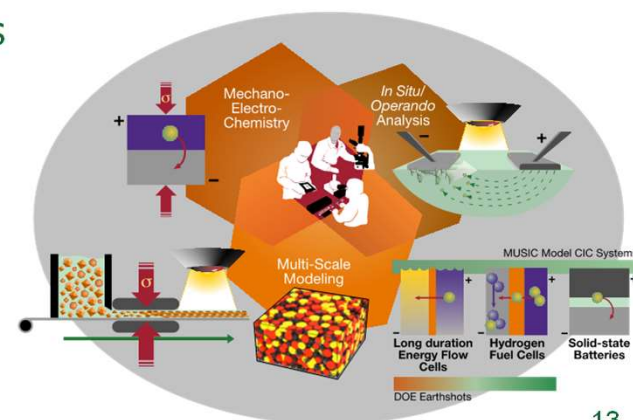
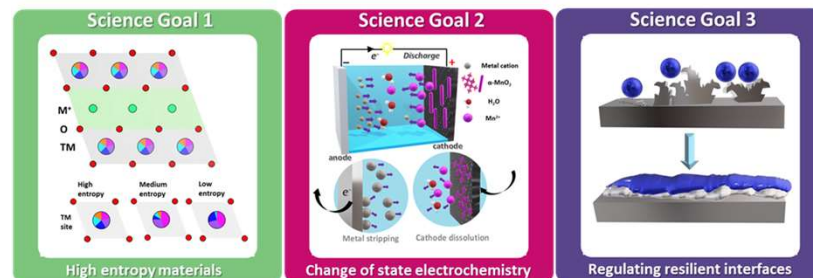


# Energy Frontier Research Centers (EFRCs)

- Coupling “basic research needs” for energy applications and “grand-challenge science”
- Bringing the academic community together with the national labs and industry to enable high-impact collaborative science with relevance to energy science

Currently 6 EFRCs performing research underpinning energy storage:

- Center for Mesoscale Transport Properties  
Esther Takeuchi (Stony Brook University)
- Mechano-Chemical Understanding of Solid Ion Conductors  
Jeff Sakamoto (University of Michigan)
- Center for Alkaline-Based Energy Solutions  
Hector Abruña (Cornell University)
- Fast and Cooperative Ion Transport in Polymer-Based Electrolytes  
Valentino Cooper (Oak Ridge National Laboratory)
- Breakthrough Electrolytes for Energy Storage and Systems  
Robert Savinell (Case Western University)
- Center for Synthetic Control Across Length-scales for Advancing Rechargeables  
Sarah Tolbert (UCLA)





# JCESR (2012-2023): Bottom-Up Battery Design

Build batteries from the bottom up

*Atomic and molecular battery design*

Extensive use of simulation and machine learning

*Materials discovery*

*Atomic/molecular level understanding*

Multi-modal experiment + simulation

*Broad range of experiments and simulations per project/paper*

Techno-economic models inform strategic choices

*System performance and cost*

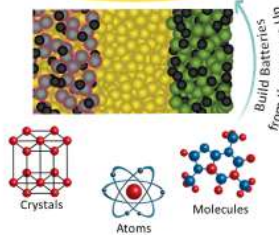
*Materials performance targets*

Industrial and community engagement

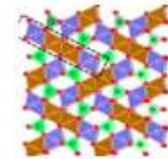
*Communicating and collaborating beyond JCESR*

## Bottom-Up Battery Design

Transformative Materials,  
Chemistries, and Architectures

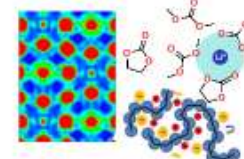


## Multivalent Ion Materials Design



Earth-abundant, higher energy density, safer, less expensive alternative to Li-ion

## Ion Solvation and Transport



Controls nearly all aspects of battery performance

## Redoxmers for Flow Batteries



Wide molecular design space for higher performance and lower cost

## JCESR's National Presence



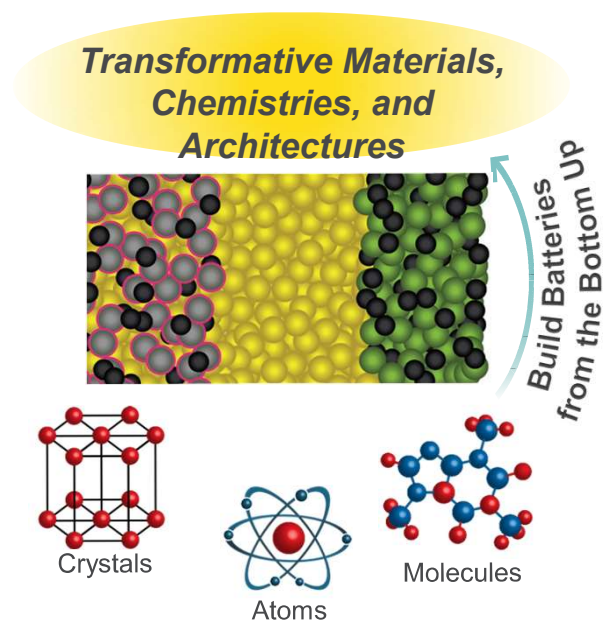


# Joint Center for Energy Storage Research (JCESR)

Venkat Srinivasan  
Argonne National Lab



ESGC Summit  
July 25, 2023



- Context for JCESR
- Vision, goals
- Enduring legacies
- Science challenges in storage



# THE ENERGY STORAGE LANDSCAPE IN 2012



Li-ion: one-size-fits-all battery  
for many applications

## Electric Vehicles and Electricity Grid

*Promising opportunities, many commercial barriers*

### Electric Vehicles

High cost, low range, no charging infrastructure, tiny market

### Electricity Grid

High cost: Battery \$825/kWh  
Battery storage: short lifetime, no deployment at scale

### JCESR Vision

Fundamental science to enable beyond Li-ion batteries  
that can meet transportation and grid targets

[Newsletters](#)**CRAIN'S** CHICAGO BUSINESS

Government

# Argonne wins Manhattan Project for car batteries

By Paul Merrion

[Reprints](#) [Share](#)

November 29, 2012 06:00 AM

Argonne National Laboratory has won federal funding for a highly coveted research center modeled after Bell Labs and the Manhattan Project that will aim to create smaller, cheaper batteries for electric vehicles and other long-range energy needs. The Energy Department's decision is expected to be announced later this week, according to two Capitol Hill sources. Argonne's Joint Center for Energy Storage Research proposal, which includes a team of four other national labs, four universities and private industry, was supported by 10 senators and 39

# GEORGE CRABTREE: THE FOUNDING DIRECTOR OF JCESR



[Home](#) > [MRS Bulletin](#) > [Article](#)

Society News | [Published: 03 April 2023](#)

## In remembrance: George Crabtree (1944–2023)

Gentleman–scientist at the forefront of sustainable energy

[Elizabeth Kócs](#), [David Cahen](#) & [Dave Ginley](#)

[MRS Bulletin](#) 48, 426–427 (2023) | [Cite this article](#)

### Scientist, visionary, and gentleman

A stunning loss to the scientific community and to humanity, the news of George Crabtree's recent demise came as a shock to his numerous colleagues and friends. George was the epitome of an inspirational visionary and an astounding human being, as well as a force for critical and interdisciplinary scientific thought. Remembered by all as approachable, warm,

# EVOLUTION OF JCESR

1. Li-S
2. Multivalent
3. Redoxmers
4. Air-breathing aq.S

Compelling  
research insights

“Bottom up” battery design

402 papers

41 inventions

2012

2018

2023

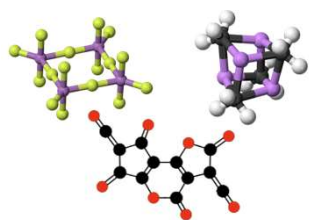




# JCESR RENEWAL VISION AND GOALS

## Three Primary Goals

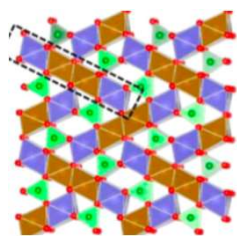
### Redoxmers for Flow Batteries



Anolytes, Catholytes and Membranes

Wide molecular design space for higher performance and lower cost

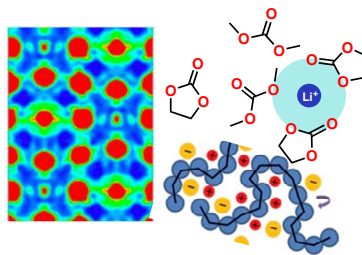
### Multivalent Ion Materials Design



Mg<sup>++</sup>, Ca<sup>++</sup>, Zn<sup>++</sup>

Material diversification to ensure supply chain security

### Ion Solvation and Transport

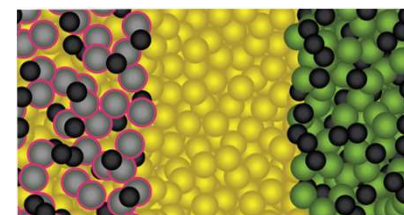


Solids, Liquids, Polymers, Membranes

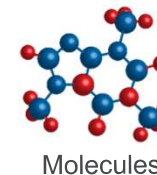
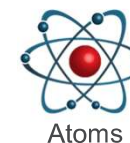
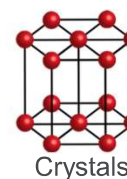
Controls nearly all aspects of battery performance

## Vision Bottom-Up Battery Design

### Transformative Materials, Chemistries, and Architectures



Build Batteries from the Bottom Up



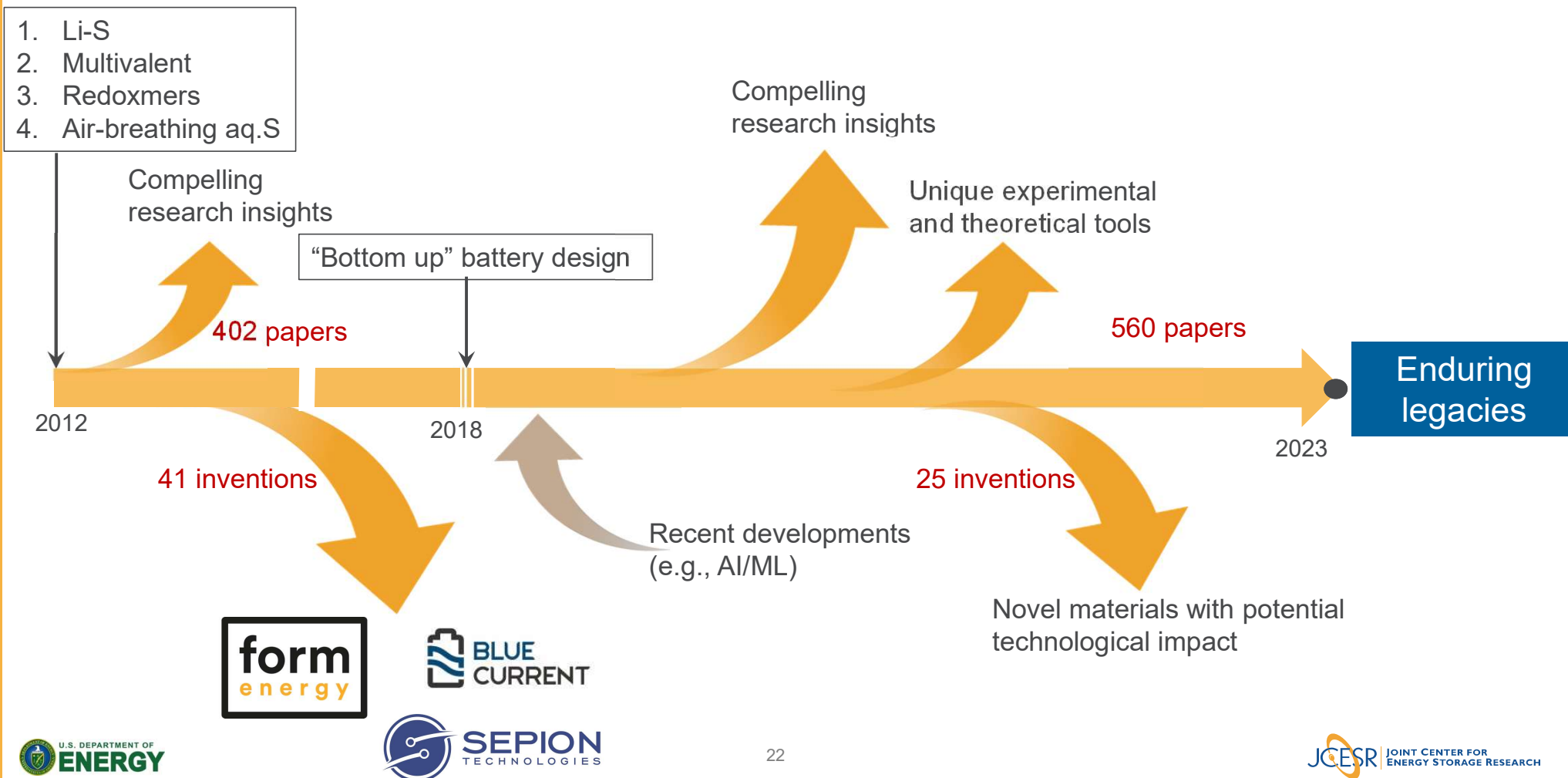
# THE TEAM



20 partners

- 6 national labs
- 13 universities
- 1 private company

# EVOLUTION OF JCESR



# JCESR ENDURING LEGACIES

## Scientific

- Ion solvation and its impact on batteries
- Divalent working ions as an enabler
- Redox active molecules (redoxmers) for storage
- Data Science, machine learning, and automated labs
- in situ, Operando characterization

## Technological

- New materials w/ technological impact
- Patents
- Spin offs
- Follow-on funding

## Operational

- Technoeconomic to guide science
- Managing team science
- Training the future workforce

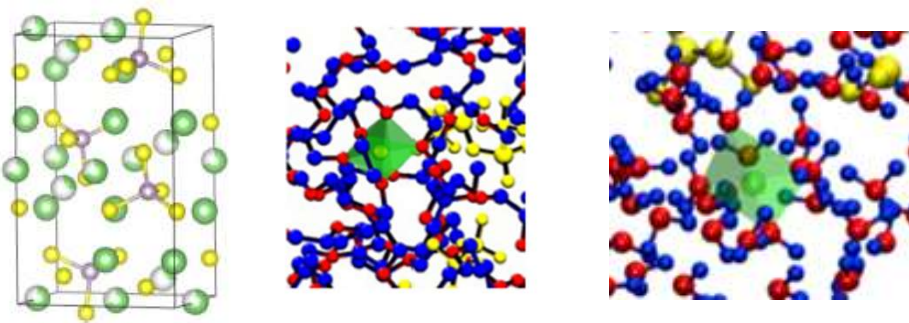


# JCESR EXTENDED THE CONCEPT OF SOLVATION FROM LIQUID ELECTROLYTES TO INORGANIC SOLIDS AND POLYMERS

Developed a common framework across phases as a guide to describe and improve ion transport

- Before JCESR, the term solvation was generally used to describe solvation shells in liquid electrolytes.
- New principles that govern the cooperative motion of ions and molecules within and outside the solvation structure (shells or cages) in all three classes of electrolytes were established.
- Discovered that theories developed first for concentrated electrolytes also apply to solid electrodes where the mobile species are ions and the electrons.

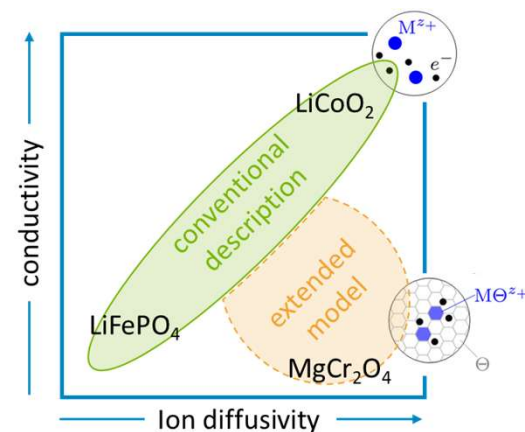
## Electrolytes Solids, Polymers, Liquids



DOI: 10.1016/j.trechm.2021.06.004  
DOI:10.1021/jacs.2c03491



## Solid Electrodes Electron – ion correlations

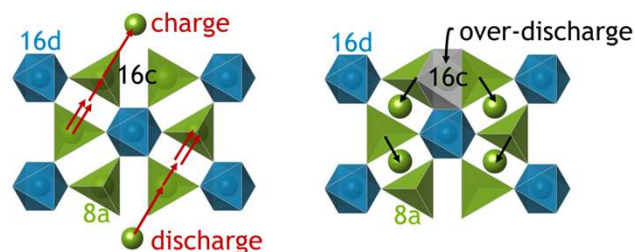


# JCESR ADVANCED THE DESIGN PRINCIPLES NECESSARY TO TRANSITION FROM MONO TO DIVALENT ENERGY STORAGE MATERIALS

Advanced divalent energy storage science by shifting focus to concerted cation motion in the solid state and cation coordination dynamics in the interfacial liquid state.

- Predictive solid-state design is advanced from conventional site-specific activation barriers to concerted charge motion through structural cation rearrangement,<sup>1</sup> cluster anion reorientation,<sup>2</sup> and coupled electron-ion transport.<sup>3</sup>
- Predictive liquid electrolyte design is advanced from conventional isolated constituent stability to controlling solvation structure at the electrode interface through coordination reconfiguration,<sup>4</sup> interfacial restructuring,<sup>5</sup> and ligand stabilization.<sup>6</sup>

**Structural cation rearrangement**  
Pushing  $M^{2+}$  reversibility limits



<sup>1</sup>Lapidus DOI 10.1021/jacs.1c04098,

<sup>2</sup>Tsai DOI 10.1002/aenm.202203284,

<sup>3</sup>Johnson & Mistry DOI 10.1021/jacs.2c03491,

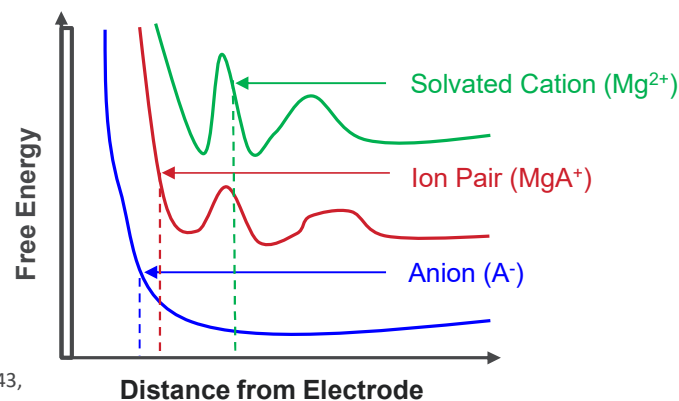
<sup>4</sup>Hahn DOI 10.1039/d0ta02502j,

<sup>5</sup>Prendergast DOI 10.1021/acs.jpcclett.1c00943,

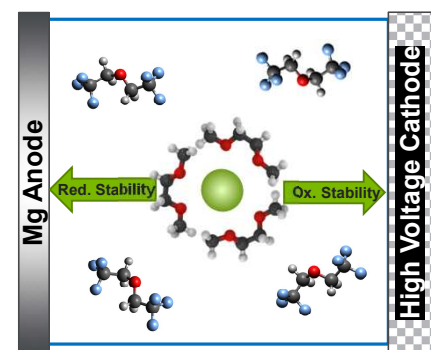
<sup>6</sup>Persson DOI 10.1021/acs.jpcc.2c06653.



**Interfacial restructuring**  
Controlling species approach



**Coordination reconfiguration**  
Stabilizing via selective solvation

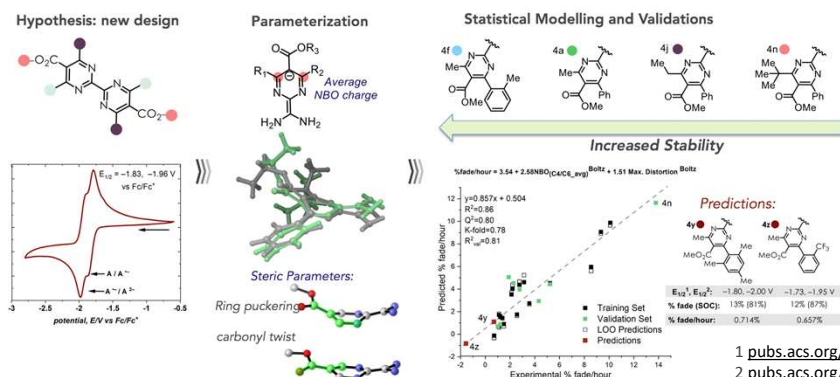


# JCESR IDENTIFIED REDOXMERS WITH EXCEPTIONAL PROPERTIES USING AN INTERDISCIPLINARY WORKFLOW

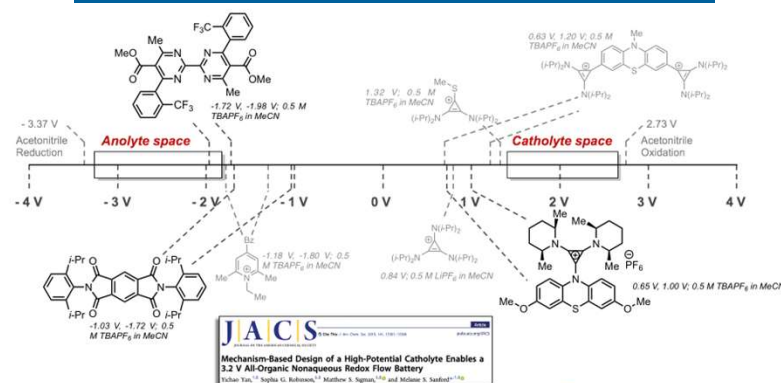
Prompted by chemical experience but perfected through synergistic experiment and computation, we downselected from millions of possibilities to few exceptional redoxmers, ultimately leading to high-performing non-intuitive designs

- Leveraged **machine learning** to design redoxmer structures displaying optimal stability,<sup>1</sup> solubility, and cross-over by funneling **thousands to millions of enumerated candidates**,<sup>2</sup> to hundreds selected for synthesis, and ultimately to few top performers, **for example enabling a 3.2 V NaRFB through high voltage, high solubility posolytes**.<sup>3</sup>
- Used a **multi-scale, multi-property characterization** toolset bolstered on X-rays, rheology, electrode dynamics, and automated characterization **alongside computational modeling** to forecast complex redoxmer interactions.<sup>4,5</sup>

Synthesis- characterization-simulation  
Workflow w/ data science



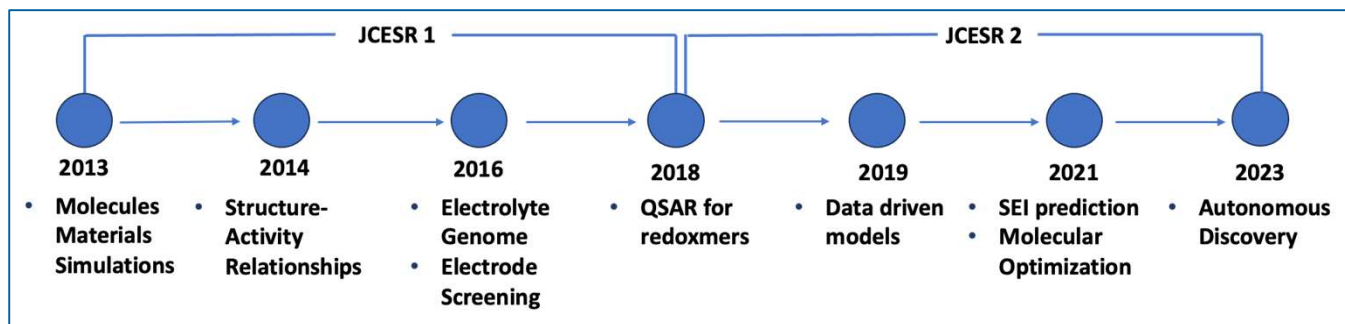
Discovery of new posolytes  
and negolytes



- [pubs.acs.org/doi/10.1021/jacs.7b00147](https://pubs.acs.org/doi/10.1021/jacs.7b00147)
- [pubs.acs.org/doi/full/10.1021/acs.chemmater.0c00768](https://pubs.acs.org/doi/full/10.1021/acs.chemmater.0c00768)
- [pubs.acs.org/doi/10.1021/jacs.9b07345](https://pubs.acs.org/doi/10.1021/jacs.9b07345)
- [www.sciencedirect.com/science/article/pii/S0167732221012575](https://www.sciencedirect.com/science/article/pii/S0167732221012575)
- [pubs.acs.org/doi/full/10.1021/acsmesuresciau.2c00054](https://pubs.acs.org/doi/full/10.1021/acsmesuresciau.2c00054)

# JCESR Utilized data-science-enhanced simulation to accelerate pace of design and discovery of Energy Storage Materials

JCESR accelerated discovery of redoxmers, electrode materials, and interfaces by developing new general and transferable ML codes, data-driven models, & autonomous electrochemical experiments.

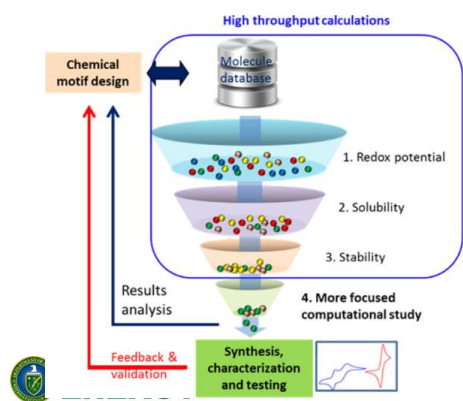


DOI: 10.1021/jz502319n

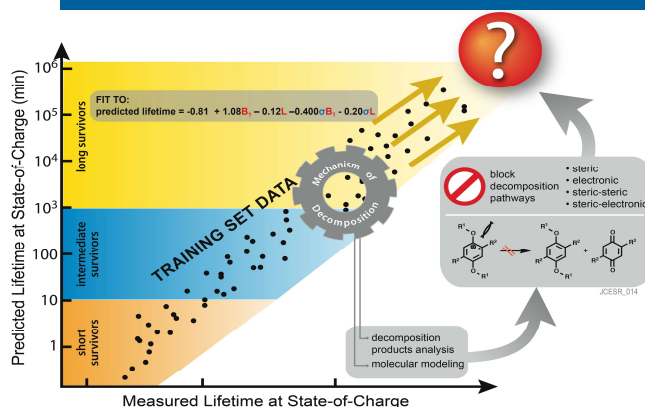
DOI: 10.1021/jacs.7b00147

DOI: 10.1021/acs.chemmater.0c00768

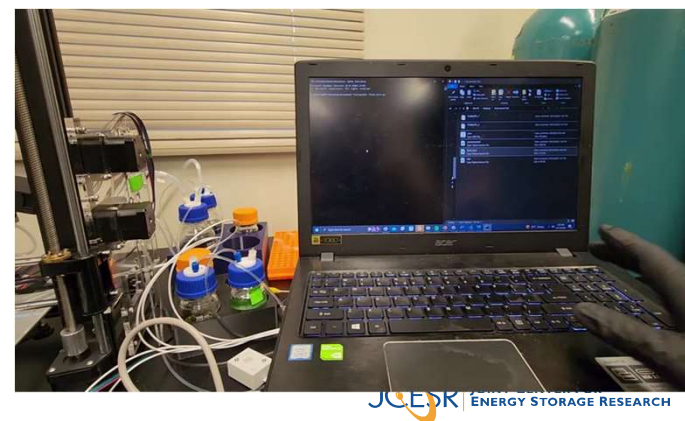
## Electrolyte Genome Database of >20k molecules



## Quantitative Structure Activity Relations Predict new molecules



## Electrolab Automated Echem lab



JCESR ENERGY STORAGE RESEARCH

# JCESR IDENTIFIED THE CRITICAL ROLE OF NEUTRAL MOLECULES IN ION TRANSPORT

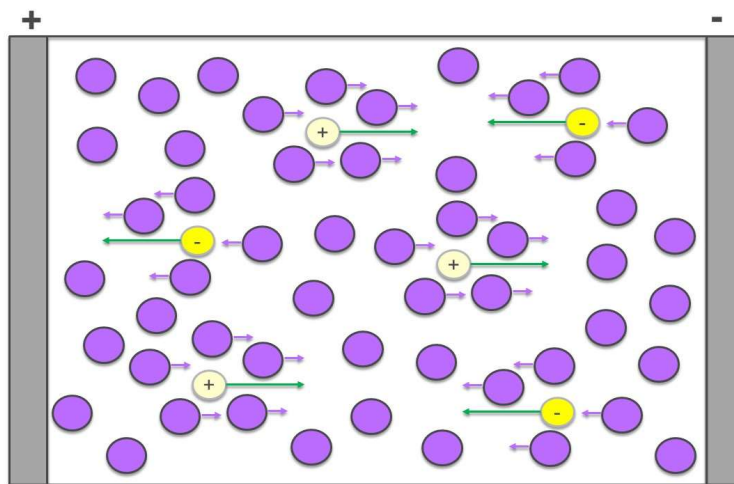
## Developed new OPERANDO TOOLS and theoretical models

- Before JCESR, electric-field-induced solvent motion was either ignored or set to zero.
- Developed operando XPCS , the only approach for measuring the velocity of neutral species under electric fields as a function of space and time. This includes solvents and polymers.
- Derived new expressions that relate solvent motion to ion transport and battery performance – they enable new interpretations of species velocities measured by eNMR.
- Showed that fast ion motion of the working ion requires neutral molecules to rapidly get out of their way.

### XPCS

measures average velocity of all solvent molecules

DOI: 10.1039/d0ee02193h  
DOI: 10.1149/1945-7111/ ac8246  
DOI:10.1103/PhysRevLett.128.198002



### eNMR

enables determination of the average velocity of solvent molecules in particular solvation shells & cages



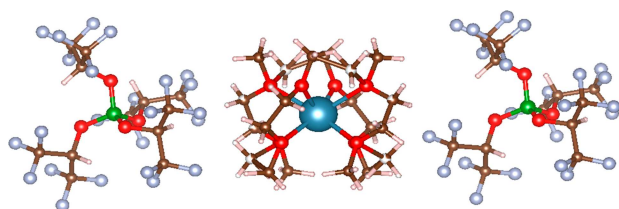
# JCESR DEVELOPED NEW ELECTROLYTES AND MEMBRANES FOR BEYOND-LITHIUM-ION TECHNOLOGIES

Developed new design and synthesis methods to advance beyond pre-JCESR bottlenecks

- Before JCESR, Ca cells cycled poorly, operated at high temperatures, and had an operating potentials below 2.6 V. The JCESR electrolyte enabled prolonged stable room temperature cycling at 3.2V.
- Optimized ion transport in polyethers, the only class of polymer electrolytes of commercial relevance.
- JCESR developed separators that have increased the capacity retention of non-aqueous redox flow batteries by 2.4 fold during 1000 charge/discharge cycles.

## Liquids

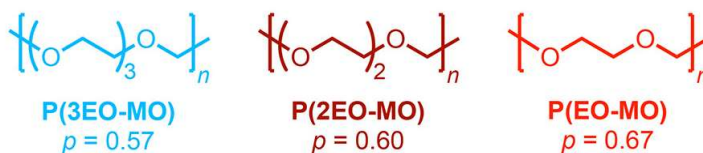
Stable electrochem window



DOI: 10.1021/jacs.1c00941  
DOI: 10.1021/acsaem.2c03836  
DOI: 10.1021/acseenergylett.2c01551

## Polymers

Optimized polyethers

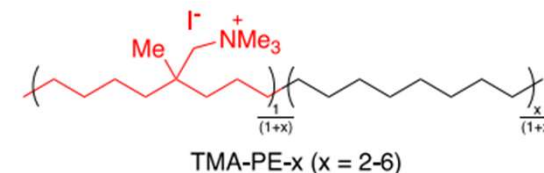


increasing  $p = \frac{[O]}{[C]}$

29

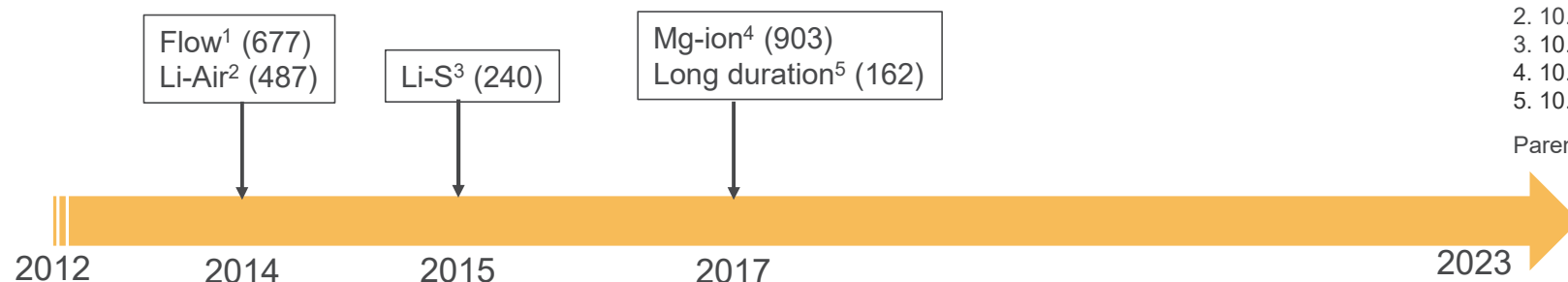
## Membranes

Eliminated crossover



# JCESR PIONEERED THE DEVELOPMENT OF DETAILED TECHNOECONOMIC MODELS FOR BEYOND LI-ION CHEMISTRIES AS A TOOL TO PRIORITIZE RESEARCH

Using technoeconomic principles, we framed the scientific challenge for the community and demonstrated the link between science and application

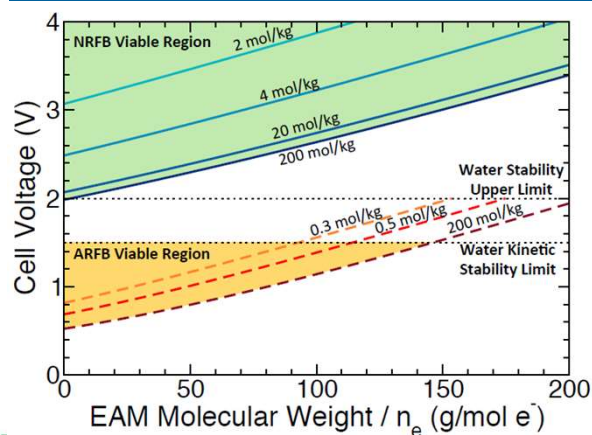


1. 10.1039/C4EE02158D
2. 10.1039/C3EE43870H
3. 10.1149/2.0611506jes
4. 10.1021/acs.chemrev.6b00614
5. 10.1016/j.joule.2017.08.007

Parenthesis denotes citations

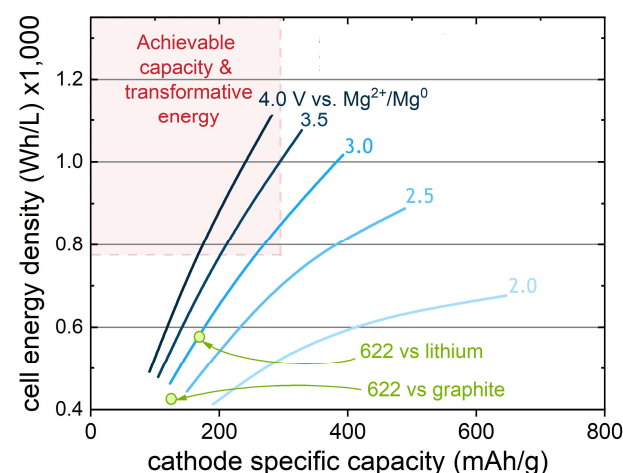
## Design space for flow batteries

Low cost aqueous and non-aqueous



## M<sup>2+</sup> cathode targets

High voltages > 3.0 V



# JCESR INSPIRED THE FORMATION OF THREE SPIN-OFF COMPANIES AND GENERATED 66 INVENTIONS, BOLSTERING US COMMERCIAL LEADERSHIP

Research nucleated in JCESR has resulted in >\$900M of follow-on funding, including >\$55M from applied offices and industry

Technology Area	Inventions (#)
Redoxmers	22
Lithium-Sulfur	6
Multivalent (Zn/Ca/Mg)	8
Solid-state/Li-metal	7

Notes: Active/available IP only. Other topics with 3 or less active technologies: Membranes, LIB Cathodes, Additives, Supercapacitors, 3D printing.

**BLUE CURRENT**



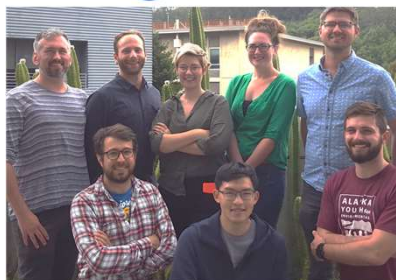
**Irene Villaluenga**  
Battery Scientist  
JCESR Alum

**Nitash Balsara**  
Co-founder  
JCESR Member

**Kevin Gao**  
Battery Scientist  
JCESR Alum

Solid state electrolytes

**SEPION TECHNOLOGIES**

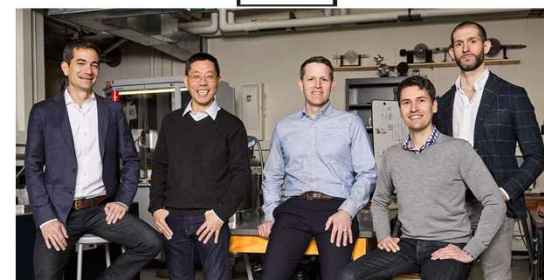


**Brett Helms**  
Co-founder  
JCESR Member

**Peter Frischmann**  
Co-founder, CEO  
JCESR Alum

Microporous polymer membranes

**form energy**



**Liang Su**  
Scientist  
JCESR Alum

**Yet-Ming Chiang**  
Co-founder  
JCESR Member

**Billy Woodford**  
CTO  
JCESR Alum

**Jarrod Milshtein**  
Senior Manager  
JCESR Alum

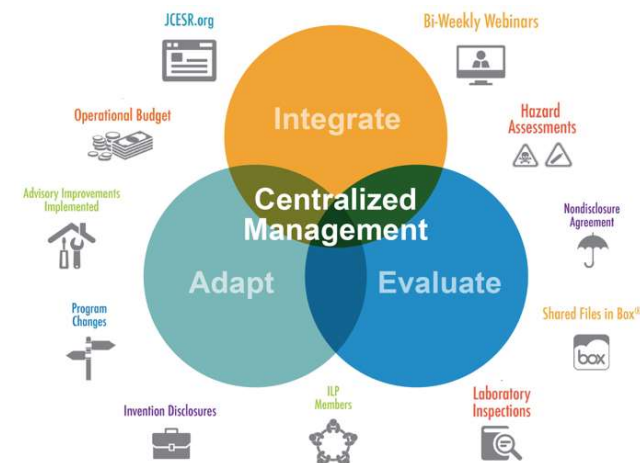
Many-day discharge batteries

# JCESR DEVELOPED AND REFINED A SUCCESSFUL MODEL FOR MANAGING TEAM SCIENCE

- JCESR management was recognized with the Secretary of **Energy's Achievement Award for Strategy and Operations in 2018**.
- JCESR developed an **Affiliates Program** and executed **13 Regional Events** (2013-2019) to engage with industrial, academic, utility, and government stakeholders across the US.
- JCESR adapted rolling wave planning and matrixed organization to manage internal milestones.
- JCESR created **Research Integration** roles to craft internal and external efforts to strengthen and promote the JCESR team within the energy storage ecosystem.



"Building a Better Battery": JCESR hosted 80 Chicago-area students and 7 teachers for full-day outreach event



## 2019 – 2023 JCESR Outreach Events

- **3 mentoring events** to encourage recruiting and diversity in STEM
- **8 scientific workshops** (2019-2022) bringing together scientific leaders and early career scientists to discuss emerging topics related to AI for energy storage, solid electrolytes, redoxmers, and the design of interfaces
- July 27, 2022 – **Identifying Energy Storage R&D Challenges for Electric Aviation** virtual workshop with RTRC to explore the fundamental electrochemical and system challenges to fully electric aviation
- April 4, 2023 – **JCESR and Beyond: Translating the Basic Science of Batteries** in-person showcase of JCESR innovation engaging the broader energy storage community



# JCESR'S 350+ EARLY CAREER ALUMNI, UNIQUELY TRAINED IN A DIVERSE AND COMPREHENSIVE RESEARCH TEAM, WILL LEAD THE GLOBAL TRANSITION TO CLEAN ENERGY



Evonik

Boğaziçi Univ.

General Motors

ORNL

Univ. of Minnesota

CO School of Mines

Argonne

Univ. of Liverpool

- JCESR graduate students and postdocs have been immersed in heavily multidisciplinary teams – imparting the **breadth of expertise** required to bring new ideas and technologies to fruition, **collaboration skills**, and extensive professional **networks**.
- JCESR supported 135 Ph.D. degrees and 221 postdocs.

## Where Are They Now?

 **53%**  
industry

 **31%**  
academia

 **12%**  
National Laboratories

**4%**  
other (government, consulting,  
venture capital, journalism)



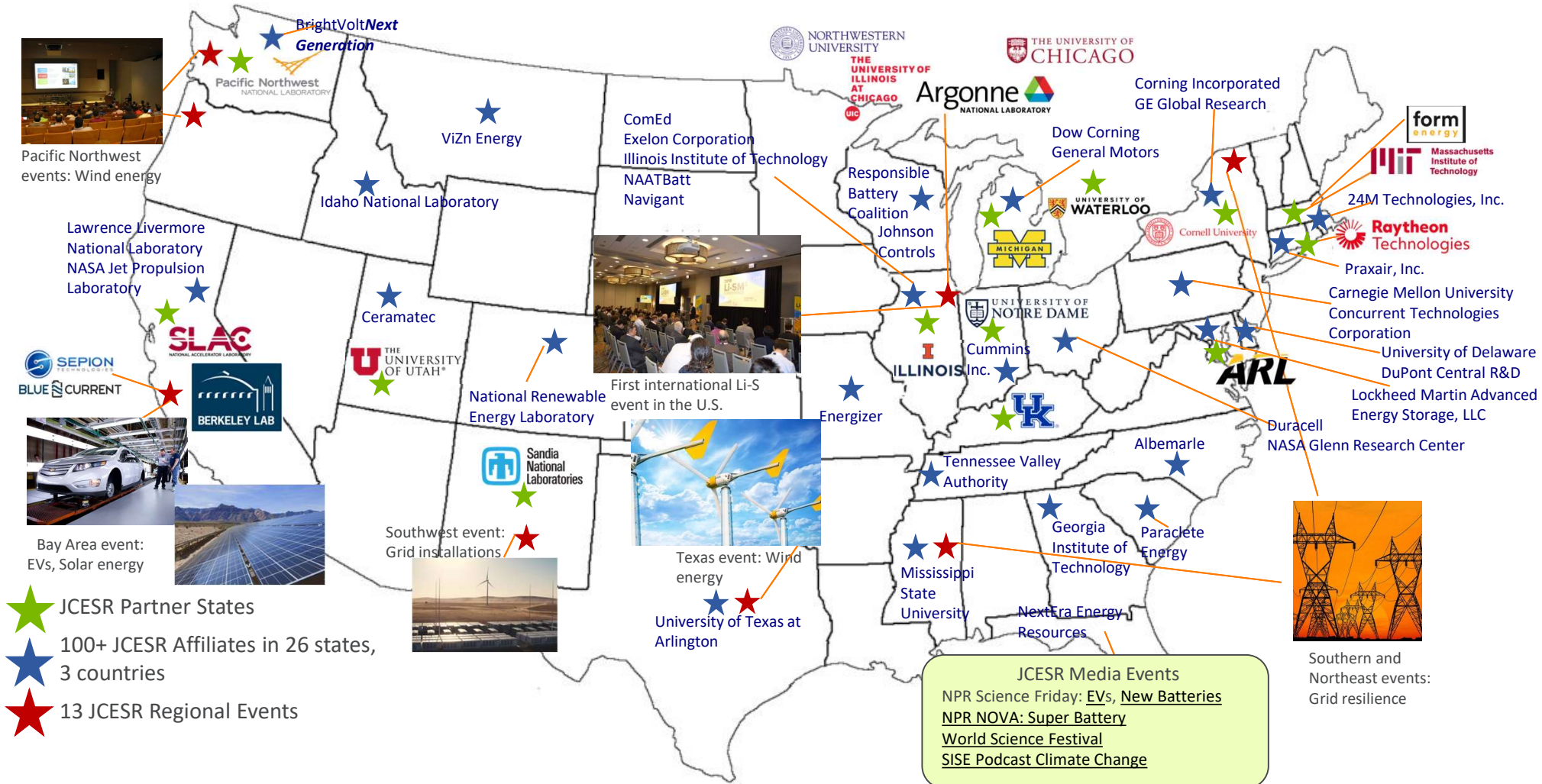
## How meaningful is/was your JCESR experience?

### Responses from the JCESR Alumni...

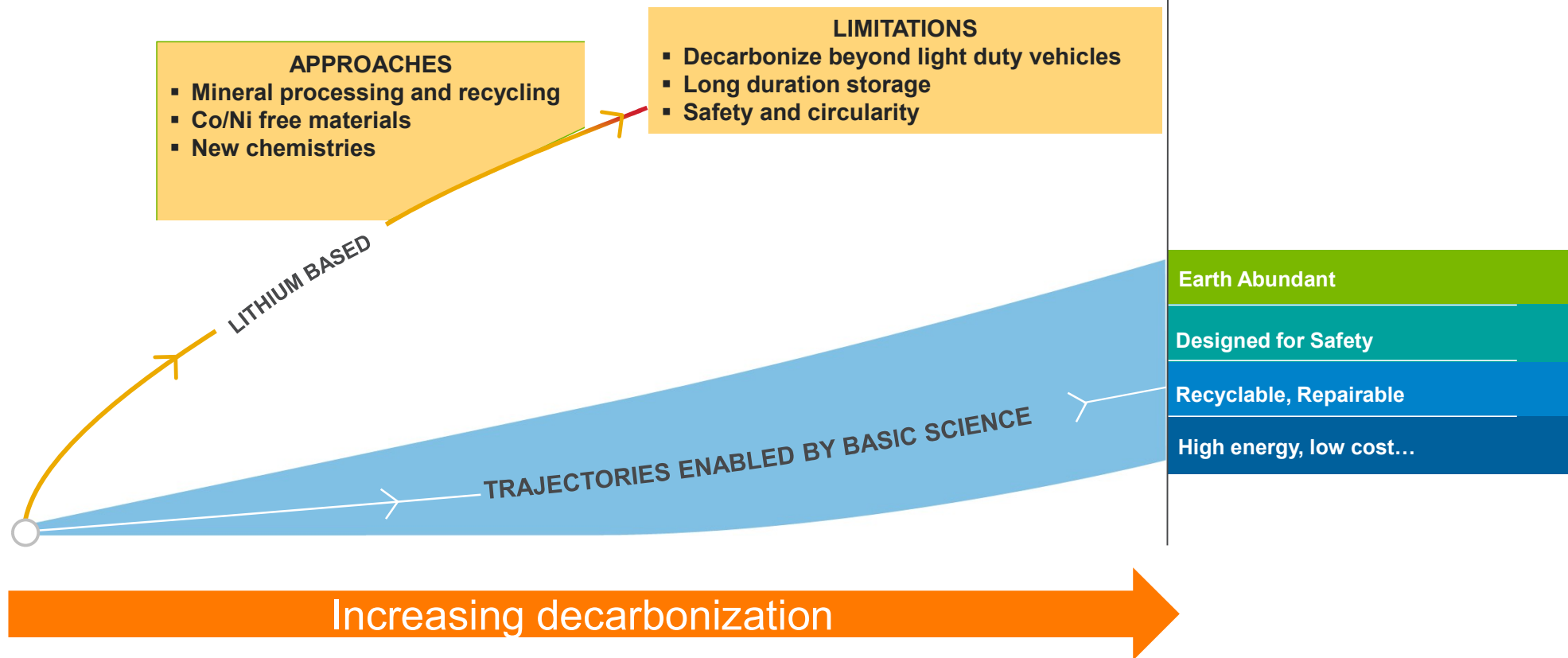
- “JCESR provided me with broad exposure to battery science and a wide spectrum of collaborators and their perspectives. It made me a better scientist.”
- “My training in JCESR was incredibly formative and allowed me to see more of the research process than I otherwise could have seen from my research group.”
- “In addition to developing applicable skills, my JCESR experience has broadened my perspective around energy technologies, providing access to knowledge and exposure to fields I may not have otherwise experienced.”
- “The network I gained has proven to be valuable over and over again. I have a strong network of folks in universities, national labs, and industry. This network has provided sources for recruiting new candidates to my team, consultant contracting work, proposal collaborators, and professional mentors.”



# JCESR'S NATIONAL REACH



# Economy wide decarbonization requires a multi-pronged approach







THANK YOU

